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THE EIGHTH ANNUAL GENERAL MEETING OF THE FARADAY DIVISION of The Chemical Society was held at 9.00 a.m. on 26 September 1979, in the Babbage Lecture Theatre, Cambridge with Professor J. S. Rowlinson M.A., D.Phil., C.Chem., F.R.I.C., F.R.S. in the Chair.

1 *Minutes*

The Minutes of the 7th Annual General Meeting which had been tabled, were approved. The Minutes were to be published in due course in the index to the 1978 Faraday Transactions.

2 *Annual Report*

The Faraday Division continued to increase its collaboration with sister Societies overseas during 1978. The spring General Discussion, sponsored jointly with the Royal Netherlands Chemical Society and held at the Conference Centre 'De Blijde Werelt', Lunteren was one such occasion and was the second Discussion to be held in The Netherlands, the first being held in Amsterdam 25 years earlier. The topic 'Colloid Stability' attracted over 260 participants of whom nearly 100 were from the U.K. with the remainder being divided almost equally between The Netherlands on the one hand and 17 other countries. The topic was proposed by the Colloid and Interface Science Group which together with the Colloid and Surfaces Group of the S.C.I. made a generous contribution towards the expenses of the meeting. The Discussion was opened by the first Rideal Lecture given by Th. G. Overbeek (University of Utrecht).

The third in the series of joint meetings with the Société de Chimie Physique, Deutsche Bunsen Gesellschaft für Physikalische Chemie and Associazione di Chimica Fisica was also held in 1978 at Fontevraud, France on the subject of 'Non-linear behaviour of molecules, atoms or ions in magnetic or electro-magnetic fields' and followed the joint meetings held in Cambridge in 1974 and in Königstein in 1976. The next joint meeting is planned for 1980 to be held in Pisa and in 1982 the Faraday Division will be responsible for a joint meeting in U.K. The Division was pleased to be able to assist a number of members with their expenses to attend the meeting.

The Second General Discussion of 1978 was held at the University of Kent at Canterbury on 'Structure and Motion in Molecular Liquids' and was sponsored by the Statistical Mechanics and Thermodynamics Group. Over 160 participants were present of whom 45% came from overseas and represented 13 countries. The Discussion was opened by the 19th Spiers Memorial Lecture given by P. A. Egelstaff (University of Guelph, Canada).

Symposium No. 13 was held in December 1978 at Queen Elizabeth College, London, on 'Pulsed Nuclear Magnetic Resonance in Solids' and was attended by 120 participants of whom 37% were from overseas representing 13 countries.

The Division took part in the Annual Congress of the Society in Liverpool with an unpublished symposium on 'The Physical Basis of Chemisorption and Heterogenous Catalysis' which was arranged in collaboration with the Surface Reactivity and Catalysis Group and convened by D. A. King and T. B. Grimley. The Divisional contribution to the Autumn Meeting at the University of Warwick comprised an informal discussion on 'Kinetics of Bimolecular Ion Molecule Reactions', convened by K. R. Jennings.

Other meetings sponsored by the Division in 1978 were 'Molecular Interactions, Microstructure and Rheological Behaviour' organised by the Industrial Sub-Committee; 'Physical Organic Chemistry' organised jointly with Perkin Division and 'Atmospheric Sensing with Lasers' organised jointly with the Institute of Physics, The Society for Chemical Industry and the Royal Meteorological Society.

The number of subject Groups affiliated to the Faraday Division increased by 2 during the year when a Group for High Resolution Spectroscopy was formed and joint sponsorship with the Institute of Physics of the Carbon and Graphite Group was approved. There are now 11 Subject Groups affiliated to the Division including 3 joint Groups with the Institute of Physics. Subject Groups continue to play an important role in the activities of the Division, not only by their involvement in General Discussions and Symposia but also by organising specialist meetings which in 1978 included the following topics:

ANNUAL GENERAL MEETING

Isotope Effects (Gas Kinetics Group)
Local Density Methods in Atomic, Molecular and Solid State Theory (Theoretical Chemistry Group)
Computers and Neutrons (Neutron Scattering Group)
Electro-Optics of Macromolecules (Polymer Physics Group)
Surface Properties of Carbons and Graphites (Carbon and Graphite Group)
Research Students' Meeting (Electrochemistry Group)
Polymer Electrets (Polymer Physics Group)
Highly Concentrated Aqueous Solutions and Molten Salts (Electrochemistry Group)
Summer School in Electrochemistry (Electrochemistry Group)
Mechanism of Catalysed Reactions (Surface Reactivity and Catalysis Group)
Structural Aspects Common to Synthetic and Biological Macromolecules (Polymer Physics Group)
International Meeting on Solid Electrolytes (Electrochemistry Group)
Fundamentals of Liquid/Liquid Interface and Emulsion Stability (Colloid and Interface Group)
Molecular Beams and Potential Energy Surfaces (Molecular Beams Group)
Energy Transfer (Gas Kinetics Group)
Recent Developments in the Chemical and Physical Characterisation of Polymers (Polymer Physics Group)
Neutron Scattering and Liquids (Neutron Scattering Group)
Organic Electrochemistry in the Chemical Industry (Electrochemistry Group)
Optical and Magnetic Properties (Theoretical Chemistry Group)
The Physical Basis of Toughness in Homogeneous Polymers (Polymer Physics Group)
Carbon and Graphite in the Aluminium Industry (Carbon and Graphite Group)
Interactions between Air Bubbles and Solid Surfaces in Liquids (Colloid and Interface Science Group)
High Resolution Spectroscopy (High Resolution Spectroscopy Group)

Professor A. Dymanus of the University of Nijmegen, The Netherlands, delivered the Bourke Lectures on 'Rotational Excitation and Population Transfer in Inter-Stellar Molecules' at Oxford and Newcastle upon Tyne and on 'Electric and Magnetic Properties of Molecules in High Resolution Spectroscopy' at the University College of North Wales, at Bangor.

Two London Symposia were sponsored by the Faraday Division in 1978, the first on 'Recent Advances in the Properties of Liquids and Solutions' which incorporated the Centenary Lecture of K. S. Pitzer and the Liversidge Lecture by J. S. Rowlinson and the second, 'Modern Spectroscopic Techniques for Studying Molecules and Ions' which incorporated the Tilden Lecture by N. B. H. Jonathan.

The Marlow Medal was awarded to R. G. Woolley of Cambridge University, distinguished for his contributions to the fundamentals of quantum electrodynamics and its relevance to chemical problems.

Newsletter No. 5 was distributed to U.K. members with the February issue of Chemistry in Britain and by mail to overseas members.

Membership of the Division in 1978 was 4376, which represented a small decrease on the 1977 membership.

3 *Treasurer's Report*

The Treasurer presented a financial statement for the 15 month period from 1 October 1977 to 31 December 1978 which was accepted.

4

Elections to Council

The members of Council elected to take office from the Society's Annual General Meeting in 1980 were as follows:

President

PROF. J. S. ROWLINSON

Vice-Presidents who have held office as President

PROF. SIR GEORGE PORTER
DR. T. M. SUGDEN
PROF. R. P. BELL

PROF. D. H. EVERETT
PROF. F. C. TOMPKINS

Vice Presidents

PROF. A. D. BUCKINGHAM
PROF. P. GRAY
PROF. G. J. HILLS
PROF. N. SHEPPARD

PROF. H. A. SKINNER
PROF. H. GG. WAGNER
PROF. D. H. WHIFFEN

Ordinary Members

DR. R. J. DONOVAN
PROF. D. A. KING
PROF. P. MEARES
DR. G. D. PARFITT
PROF. J. H. PURNELL

DR. J. P. SIMONS
PROF. F. S. STONE
PROF. F. L. SWINTON
PROF. M. C. R. SYMONS
PROF. J. M. THOMAS

Honorary Secretary

PROF. G. J. HILLS

Honorary Treasurer

PROF. P. GRAY

5 *Review of Future Activities*

The President drew attention to the programme of future activities of the Division, which had been tabled. In 1982 the fifth in the series of joint meetings with the Deutsche Bunsen Gesellschaft für Physikalische Chemie, the Société de Chimie Physique and the Associazione Italiana di Chimica Fisica was due to be held in the U.K., organized by the Faraday Division, and members were invited to suggest topics for this meeting.

NOTICES TO AUTHORS—No. 7/1970

Deposition of Data—Supplementary Publications Scheme

Preamble

The growing volume of research that produces large quantities of data, the increasing facilities for analysing such data mechanically, and the rising cost of printing are each making it very difficult to publish in the *Journal* in the normal way the full details of the experimental data which become available. Moreover, whilst there is a large audience for the general method and conclusions of a research project, the number of scientists interested in the details, and in particular in the data, of any particular case may be quite small. The British Library Lending Division (B.L.L.D.) in consultation with the Editors of scientific journals, has now developed a scheme whereby such data and detail may be stored and then copies made available on request at the B.L.L.D., Boston Spa. The Chemical Society is a sponsor of this scheme and has indicated to the B.L.L.D. its wish to use the facilities being made available in this "Supplementary Publications Scheme".

Bulk information (such as crystallographic structure factor tables, computer programmes and output, evidence for amino-acid sequences, spectra, etc.), which accompany papers published in future issues of the Chemical Society's *Journal* may in future be deposited, free of charge, with the Supplementary Publications Scheme, either at the request of the author and with the approval of the referees or on the recommendation of referees and the approval of the author.

The Scheme

Under this scheme, authors will submit articles and the supplementary material to the *Journal* simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication the supplementary material will be sent by the Society to the B.L.L.D. where it will be stored. Copies will be obtainable by individuals both in the U.K. and abroad on quoting a supplementary publication number that will appear in the parent article.

Preparation of Material

Authors will be responsible for the preparation of camera-ready copy according to the following specifications (although the Society will be prepared to help in case of difficulty).

- (a) Optimum page size for text or tables in typescript: up to 30 cm × 21 cm.
- (b) Limiting page size for text or tables in typescript: 33 cm × 24 cm.
- (c) Limiting size for diagrams, graphs, spectra, etc.: 39 cm × 28.5 cm.
- (d) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.
- (e) Pages should be clearly numbered.

It is recommended that all material which is to be deposited should be accompanied by some prefatory text. Normally this will be the summary from the parent paper and authors will greatly aid the deposition of the material if a duplicate copy of the summary is provided. If authors have the facilities available the use of a type face designed to be read by computers is encouraged.

Deposition

The Society will be responsible for the deposition of the material with the B.L.L.D. The B.L.L.D. will not receive material direct from authors since the Library wishes to ensure that the material has been properly and adequately refereed.

Action by the Society

The Society will receive a manuscript for publication together with any supplementary material for deposition and will circulate all of this to referees in the normal way. When the edited manuscript is sent to the printers the supplementary material will be sent for deposition to the B.L.L.D. who will issue the necessary publication number. The Society will add to the paper, at the galley proof stage, a footnote indicating what material has been deposited in the Supplementary Publications Scheme, the number of pages it occupies, the supplementary publication number, and details as to how copies may be obtained.

Availability

Copies of Supplementary Publications may be obtained from the B.L.L.D. on demand by organisations which are registered borrowers. They should use the normal forms and coupons for such requests addressing them as follows:

Mr. J. P. Chillag,
British Library Lending Division,
Boston Spa,
Wetherby,
West Yorkshire, LS23 7BQ, U.K.

Non-registered users may also obtain copies of Supplementary Publications but should first apply for price quotations. These are available from the Loans Office at the above address.

In all correspondence with the B.L.L.D. or the Society authors must cite the supplementary publication number.

International Collaboration

A similar scheme (known as the National Auxiliary Publications Service) is being operated in the U.S.A. by the American Society for Information Science. Similar schemes are also being contemplated in other countries. The provision of reciprocal arrangements for the exchange of supplementary data between the various national deposition centres is being investigated.

NOTICE TO AUTHORS—No. 9/1974

Nomenclature

For many years the Society has actively encouraged the use of standard I.U.P.A.C. nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Although the I.U.P.A.C. rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general.

In order to encourage authors to use I.U.P.A.C. nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given.

'Nomenclature of Organic Chemistry, Sections A, B, and C', Butterworths, London, 2nd Edition, 1971.

'Nomenclature of Inorganic Chemistry', Butterworths, London, 1971.

'Manual of Symbols and Terminology for Physicochemical Quantities and Units', Butterworths, London, 1970.

In addition to the above publications, provisional rules for the naming of organometallic compounds, amino-acids, carbohydrates, carotenoids and steroids, and rules of stereochemistry are available from the:

I.U.P.A.C. Secretariat,
Bank Court Chambers,
2-3 Pound Way,
Cowley Centre,
OXFORD OX4 3YF.

It is recommended that where there are no I.U.P.A.C. rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff.

NOTICE TO AUTHORS—No. 10/1976

Authentication of New Compounds

(1) It is the responsibility of authors to provide fully convincing evidence for the homogeneity and identity of all compounds they claim as new. Evidence of both purity and identity is required to establish that the properties and constants reported are those of the compound with the new structure claimed.

(2) In the context of this Notice a compound is considered as new (*a*) if it has not been prepared before, (*b*) if it has been prepared before but not adequately purified, (*c*) if it has been purified but not adequately characterised, (*d*) if, earlier, it has been assigned an erroneous constitution, or (*e*) if it is a natural product synthesised for the first time. In preliminary communications compounds are often recorded with limited characterising data; in spite of (*c*) above later preparations of such compounds are not considered as new if the properties previously reported are confirmed; the same applies to patents.*

(3) Referees are asked to assess, as a whole, the evidence in support of the homogeneity and structure of all new compounds. No hard and fast rules can be laid down to cover all types of compounds, but the Society's policy remains unchanged in that evidence for the unequivocal identification of new compounds should normally include good elemental analytical data; an accurate mass measurement of a molecular ion does not provide evidence of purity of a compound and must be accompanied by independent evidence of homogeneity. Low-resolution mass spectroscopy must be treated with even more reserve in the absence of firm evidence to distinguish between alternative molecular formulae. Where elemental analytical data are not available, appropriate evidence which is convincing to an expert in the field will be acceptable, but authors should include, for the referees, a brief explanation of the special nature of their problem.

(4) Spectroscopic information necessary to the assignment of structure should normally be given. Just how complete this information should be must depend upon the circumstances; the structure of a compound obtained from an unusual reaction or isolated from a natural source needs much stronger supporting evidence than one derived by a standard reaction from a precursor of undisputed structure. Authors are reminded that full spectroscopic assignments may always be treated as a Supplementary Publication where their importance does not justify their inclusion in the published paper.

(5) Finally, referees are reminded of the need to be exacting in their standards but at the same time flexible in their admission of evidence. It remains the Society's policy to accept work only of high quality and to permit no lowering of present standards.

* New compounds should be indicated by underlining the name (for italics) at its first mention (excluding headings) in the Experimental section only, and by giving analytical results in the form: (Found: C, 63.1; H, 5.4. $C_{13}H_{13}NO_4$ requires C, 63.2; H, 5.3 %). If analytical results for compounds which have been adequately described in the literature are to be included, they should be given in the form: (Found: C, 62.95; H, 5.4. Calc. for $C_{13}H_{13}NO_4$: C, 63.2; H, 5.3 %). Analyses are normally quoted to the nearest 0.05 %.

Publication of Theoretical and Computational Papers

The Primary Journals Committee has been considering future policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programs. Many such papers report what would be considered 'routine work' in other areas of chemistry and have often included extensive detail.

A specialist sub-committee formulated a set of proposals which were circulated to a large representative sample of theoretical chemists and met with general acceptance. These, with the comments on them, form the basis of this notice.

The Primary Journals Committee recognises that computational work can play a valuable role in chemistry, and will probably continue to do so on an increasing scale. It accepts the time-honoured principle that the first criterion for publication of a paper by the Society should be the worthiness of the chemical problem considered, rather than the particular techniques employed by the author. For example, the use of a new computing algorithm, or the modification of a program, would not usually, on its own, provide sufficient justification for publication.

The Primary Journals Committee recommends to authors the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

- (i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to Faraday Transactions II, one in which the computations are incidental to the chemistry to Perkin, Dalton or Faraday I Transactions. Papers concerned mainly with computational details are unlikely to be accepted.
- (ii) The purpose of the paper and the precise objectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.
- (iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer program used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.
- (iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.

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